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A Numerical Methodology For The Multi-Objective Optimization Of The DI Diesel Engine Combustion

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Abstract

DI Diesel engine are widely used both for industrial and automotive applications due to their durability and fuel economy. Nonetheless, increasing environmental concerns force that type of engine to comply with increasingly demanding emission limits, so that, it has become mandatory to develop a robust design methodology of the DI Diesel combustion system focused on reduction of soot and NOx simultaneously while maintaining a reasonable fuel economy. In recent years, genetic algorithms and CFD three-dimensional combustion simulations have been successfully applied to that kind of problem. However, combining GAs optimization with actual CFD three-dimensional combustion simulations can be too onerous since a large number of calculations is usually needed for the genetic algorithm to converge, resulting in a high computational cost and, thus, limiting the suitability of this method for industrial processes. In order to make the optimization process less time-consuming, CFD simulations can be more conveniently used to generate a training set for the learning process of an artificial neural network which, once correctly trained, can be used to forecast the engine outputs as a function of the design parameters during a GA optimization performing a so-called virtual optimization.

In the current paper, a numerical methodology for the multi-objective virtual optimization of the combustion of an automotive DI Diesel engine, which relies on artificial neural networks and genetic algorithms, was developed.

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Keywords: artificial neural networks, genetic algorithm, multi-objective optimization, DI Diesel engine

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Nomenclature

ANN	Artificial neural network
RBF	Radial basis function
GA	Genetic algorithm
CFD	Computational fluid dynamics
ICE	Internal combustion engine
DI	Direct injection
IMEP	Indicated mean effective pressure
CA	Crank angle
TDC	Top dead center
ATDC	After top dead center
CR	Compression ratio
SR	Swirl ratio
MFB	Burnt fuel mass
RNG	Renormalisation group
SOI	Start of injection
HSOI	Hydraulic start of injection
λ	Air/fuel equivalence ratio
Φ	Fuel/air equivalence ratio
κ	Turbulent kinetic energy
ϵ	Eddy dissipation rate

1. Introduction

DI Diesel engine are widely used both for industrial and automotive applications due to their durability and fuel economy. However, increasing environmental concerns force that type of engine to comply with increasingly demanding emission limits. Over the years, both NO_x and soot emission have been drastically decreased and the upcoming Euro6 emission standard is even more pressing, so that, although Diesel engine are more and more equipped with one or more after-treatment devices, a significant combustion improvement is needed to meet the latest emission standards. In such a scenario, it has become mandatory to develop a robust design methodology of the DI Diesel combustion system focused on reduction of soot and NO_x simultaneously while maintaining a reasonable fuel economy.

With the current status of CPU speed and model development, combustion modeling of the DI Diesel engine by means of a CFD code is becoming a necessary tool to optimize the Diesel combustion system, both in terms of emissions and performance, allowing to investigate a large number of possible configurations in a very short time, thus, overcoming limitations and drawbacks of experimentally executed parametric searches which need huge expenses and huge time. Nonetheless, since there are trade-off relationships between engine performance, NO_x and soot emissions, numerically executed parametric searches can not find a unique solution which optimizes all the objectives of a good design at the same time but rather there will exist different solutions, all representing an efficient allocation of resources, known as Pareto optimal solutions.

To overcome these issues, the design of an efficient DI Diesel combustion system can no longer rely exclusively upon experience, but rather should be mathematically represented as a multi-objective optimization problem, the objectives being the minimization of NO_x and soot emissions and the maximization of engine performance, for which multi-objective genetic algorithms and CFD calculations have been successfully applied in recent years.

At University of Wisconsin-Madison several studies on Diesel optimization have been conducted.

In [1] Senecal et al. developed a computational methodology for engine design using multi-dimensional spray and combustion modeling. The KIVA-GA code incorporated an improved KIVA-3V CFD model within the framework of a μ GA optimization technique. The design factors were: boost pressure, EGR level, start of injection, injection

duration, mass in the first pulse, dwell between pulses The μ GA efficiently determined a set of input parameters resulting in significantly lower soot and NO_x emissions compared to the baseline case.

In [2] a non-dominated sorting algorithm (NSGA-II) was coupled the KIVA CFD code, as well as with an automated grid generation technique to conduct the multi-objective optimization with goals of low emissions and improved fuel economy. The study identifies the aspects of the combustion and pollutant formation that are affected by mixing, and offers guidance for better matching of the piston geometry with the spray plume for enhanced mixing.

In [3] Shrivastava et. al performed a full engine cycle simulation within the framework of a genetic algorithm code. A 1-D gas dynamics code was used for the simulation of the gas exchange process, coupled with the KIVA-GA code for the three-dimensional simulation of spray, combustion and emission formation.

In [4] Wickman et al. used the KIVA-GA methodology to optimize the engine performance using nine input variables simultaneously. Three chamber geometry related variables were used along with six other variables, which were thought to have significant interaction with the chamber geometry.

In [5] Brahma et al. performed an optimization of some relevant engine parameters using a set of neural networks, trained on a multi-dimensional CFD code to predict pressure, torque and emissions.

Doshisha University has focused on the multi-objective optimization of the Diesel engine using genetic algorithms and a phenomenological model [6]. The HIDECS model [7], which is based on the phenomenological model, was used. An extended GA that is called the Neighbourhood Cultivation Genetic Algorithm (NCGA) was used. The NCGA has the neighbourhood crossover mechanism besides the mechanism of NSGA-II [8].

Research activities at University of Salento cover the multi-objective GA optimization of the DI Diesel engine combustion chamber and of the common rail injector. In [9] a GA optimization of some geometric features of the combustion chamber was performed. For all the investigated chambers, bowl volume and squish-to-volume ratio were kept constant in order to ensure the same compression ratio. The evaluation phase of the genetic algorithm was performed by simulating the behaviour of each chamber with a modified version of the KIVA-3V code. The optimization method was based on the use of genetic programming, a search procedure developed at the University of Michigan.

In [10] the same optimization method was applied to the optimization of a common rail injector. Three different methods, based on variable weights combination, distance from the global optimum and individuals' rank respectively, were implemented for the calculation of the overall fitness. The optimization aimed at identifying the values of seven geometrical parameters which gave a needle lift law as close as possible to the current impulse governing the injection event.

2. Contribution

Several authors have proposed different methodologies relying upon multi-objective genetic algorithms for the optimization of the DI Diesel engine and have shown the effectiveness of that mathematical approach. However, multi-objective genetic algorithm optimizations in which the evaluation phase is entirely demanded to CFD calculations make the optimization procedure time-consuming since a large number of calculations is needed for the genetic algorithms to converge. On the contrary, when the evaluation phase of the genetic algorithm relies upon phenomenological models, though computational costs are greatly decrease, serious limitations are faced while investigating piston bowl change-in-shape and the accuracy of the model strongly depends upon its experimental validation.

The aim of the current study was to develop and validate a hybrid approach for the multi-objective optimization of the DI Diesel engine which was, at the same time, fast and accurate. At the base of the methodology, three-dimensional CFD calculations were used to generate a valid training set for the learning process of an artificial neural network. Artificial neural network were chosen amongst other statistical modeling tools due to their ability to model complex relationships between inputs and outputs like those which tie up design parameters and objectives inside the DI Diesel engine. Then, once properly trained, the artificial neural networks were used during the evaluation phase of the genetic algorithm to foresee NO_x, soot and gross-IMEP as a function of the input parameters. The NSGA-II genetic algorithm [8] was used due to its ability to find Pareto optimal solutions in one single run with a low computational cost. At the final stage, only the best individuals were verified through actual three-dimensional CFD simulations and a deep investigation of their combustion development was carried out.

3. Investigated engine

In the present study, the numerical methodology for the multi-objective optimization was used to aid the design process of a VM Motori DI Diesel engine targeted for automotive applications. The investigated engine was a 4-valve for cylinder engine whose main specifications are reported in table 1.

Table 1. Engine specifications

Bore [mm]	Stroke [mm]	Conrod [mm]	CR	Squish height [mm]	Regime [rpm]
92	92	159	15.5	0.7	4000



Fig. 1. (a) Piston bowl A; (b) Piston bowl B; (c) Piston bowl C;

During the development process of the engine, three different piston bowls (figure 1) were tested. All the piston bowls had the same volume resulting in a compression ratio of 15.5. The piston bowl A was the baseline design of engine while the other two piston bowls were designed with quite different shape in order to develop different combustion concepts and, thus, could need different operating conditions as optimal conditions.

The reference injection strategy of investigated operating condition is reported in table 2.

Table 2. Injection strategy

HSOI [deg. ATDC]	Duration [deg.]	Rail pressure [bar]	Inj. mass [mg/stroke]	Inj. holes	Spray angle[deg.]	Delivery rate [$\text{cm}^3/30\text{s}$]
-9.0	40.0	2000	76.5	7	74	400

4. CFD combustion simulations models

The CFD code KIVA3D, a modified version of the KIVA-3 code [11] developed at the University of Bologna since 1996, was used to perform the in-cylinder combustion simulations. The turbulence RNG k-eps linear model model has been updated following the work of Han et al. [12], and Bianchi et al. [13]. The fuel liquid dispersed phase is treated according a Lagrangian approach using the hybrid spray breakup model proposed and validated by Bianchi and Pelloni [14]. The latter accounts for both the atomization of the liquid jet and the droplet secondary breakup. The spray-wall interaction was modelled according to Cazzoli et al. [15]. The fuel auto-ignition is simulated using the Shell model in the implementation proposed by Kong et al. [16]. The high-temperature combustion part follows the characteristic-time combustion model developed by Abraham et al. [17], with the correction proposed by Bianchi et al. [18] to account for non-equilibrium turbulence effects of the energy cascade and thus on the turbulence time scales. Finally the extended Zeldovich mechanism is used to model NO_x formation while the Hiroyasu's formation model [7] and the Strickland-Constable's model for the oxidation [19] have been used to predict in-cylinder soot.

As far as the combustion calculations are concerned, the initial in-cylinder pressure and temperature at IVC have been evaluated accounting for the internal EGR following Senecal et al. [20] based on the target boost pressure, the external

EGR rate and the air-to-fuel ratio. The in-cylinder pressure and the species densities have been assumed to be uniform at the beginning of the computation at the intake valve closure.

The hydraulic injection profile has been defined according to the target ECU controlling data (SOI, excitation time, injection pressure) using a modified version of the AMESim model developed by Bianchi et Al. [21].

CFD calculations were performed on a sector of 51.43 degrees of the whole computational domain, exploiting the axi-symmetry of both geometry and flow, in order to reduce the computational costs of the combustion concept development [22]

5. RBF neural networks

A radial basis function (RBF) neural network is a special type of feed-forward neural network that uses a radial basis function defined as its activation function and is composed of three layer: the input layer, the hidden layer and the output layer as shown in figure 2.

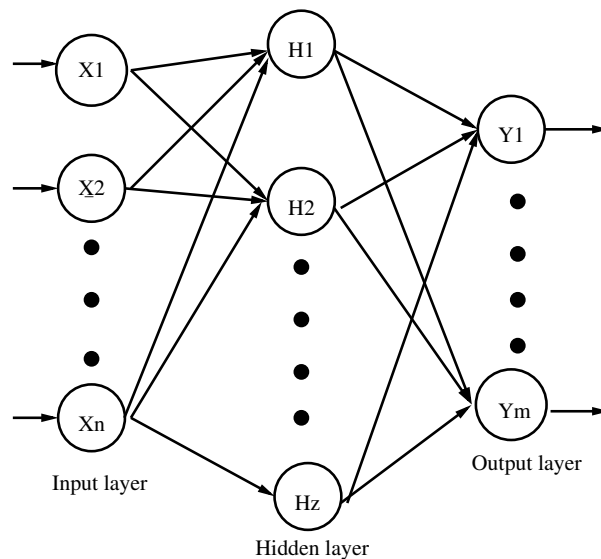


Fig. 2. RBF neural network lay-out

The input layer relies on as many neurons as input features. Input neurons just propagate input features to the next layer.

The hidden layer is composed of a number of neurons m_1 which must be lower or equal to N , where N is the number of training set data. Each neuron in the hidden layer is associated with a kernel function, in our case a Gaussian radial basis function, defined as:

$$G(x, x_i) = \exp\left(-\frac{1}{2\sigma_i^2} \|x - x_i\|^2\right) \quad (1)$$

where x_i is the center of the kernel function and σ_i its width.

The output layer is composed of as many neurons as the outputs of the observed system. Each output neuron is the weighted sum of the hidden layer functions defined as follows:

$$F(x) = \sum_{i=1}^{m_1} w_{ij} G(x, t_i) \quad (2)$$

where w_{ij} — $i = 1, 2, \dots, m_1$ are the weights of each hidden neuron.

6. Neural networks learning

The learning strategy of the RBF neural network was performed in two different steps according to [23]:

1. the hidden layer was trained by selecting the centers and widths of the kernel functions associated with the hidden neurons. Centers were selected using a *K-means* clustering technique [24]. Widths were defined using the the *p-nearest neighbor* (p-nn) algorithm [25].
2. the weights corresponding to the connections between the hidden neurons and the output neurons were defined by solving the set of linear equations given by a pseudo-inverse matrix [26].

A full-factorial design of experiment of 81 CFD three-dimensional combustion calculations was simulated, starting from the values of the input variables P_{boost} , SR, EGR SOI reported in table 3, for each investigated piston bowl in order to provide an adequate training set for the learning processes of the radial basis functions neural networks.

The computational cost needed to simulate each training set was about 24 hours on a 8 Intel Xeon core @ 2.4 GHz computer. Input parameters were chosen, as reported in table 3, in order to focus the optimization of the engine on the variables which were more strongly related to design choices. P_{boost} represented the in-cylinder pressure at intake valve closure. SR was the swirl ratio at intake valve closure. EGR was the in-cylinder exhaust gas mass fraction at intake valve closure. SOI was referred to the hydraulic start of injection. The range of each input variable was chosen to ensure a wide exploration of the design space.

Training sets of the piston bowls A, C, B were kept separated to train different neural networks for each piston bowl allowing to clearly separate the influence of the piston shape, which affect the spray/wall interaction, from the influences of the other input variables.

Table 3. Input parameters ranges

P_{boost} [bar]	SR [-]	EGR [%]	SOI [deg. ATDC]
3.25	1.0	5.0	-6.0
3.32	1.5	10.0	-9.0
3.39	2.0	15.0	-12.0

In order to validate the neural networks and to verify their ability to forecast engine performance and emissions as a function of the input variables, the training sets of each piston bowl were divided into two different parts: the first part of each training set, composed of 78 data, was used to train the related neural network. The remaining part of each training set, composed of 3 data, was instead use to validate the related neural network.

Figure 3 shows the relative error between the foreseen values of NOx, soot and gross-IMEP of the neural networks and the actual ones of the validation sets.

As it can be seen, all the trained neural networks evaluated the engine gross-IMEP with a very good precision (the highest relative error was 1.5%) while the evaluation of engine emissions recorded higher relative errors varying from about 2% through about 8%.

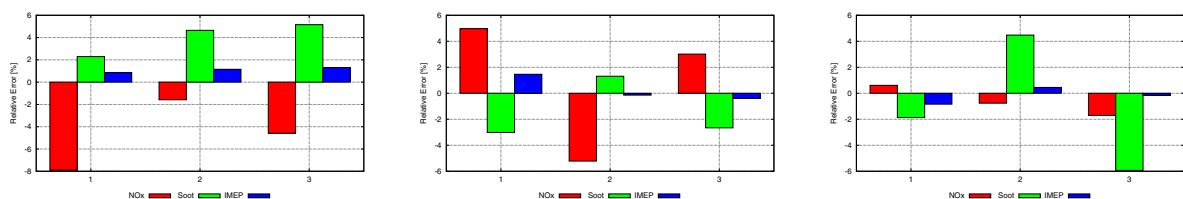


Fig. 3. (a) A neural network validation; (b) B neural network validation; (c) C neural network validation

7. Multi-objective optimization of the piston bowls

After the learning process, a multi-objective genetic algorithm virtual optimization was performed for each piston bowl.

The non dominated sorting genetic algorithm NSGA-II [8] was used since the optimal solutions of the DI Diesel combustion engine are the non dominated ones, being NO_x, soot and gross-IMEP linked together by trade-off relationships.

For each optimization an initial population of 72 individuals, randomly generated, was used as the first generation of an evolutionary process which advanced through 100 generations virtually examining, by means of the RBF neural networks, 7200 possible configurations in less than 2 minutes while a GA optimization fully based on actual CFD three-dimensional CFD calculations would have required approximately 2100 hours on a 8 Intel Xeon core @2.40 GHz computer.

Figures 4 (a), 5 (a), 6 (a) show how the emissions in the soot-NO_x plane, of each investigated individual for the piston bowls A, B and C respectively.

At the end of the optimization process, it was possible to define the Pareto frontier of all the three piston bowls.

It is worth noting that, although the optimization had three different objectives (minimizing NO_x and soot emissions and maximizing the gross-IMEP), it was chosen to represent the Pareto frontier in the soot-NO_x plane due to the fact that in industrial applications emissions are usually a more pressing commitment than the achievement of the power target of the engine which is, though, still desirable.

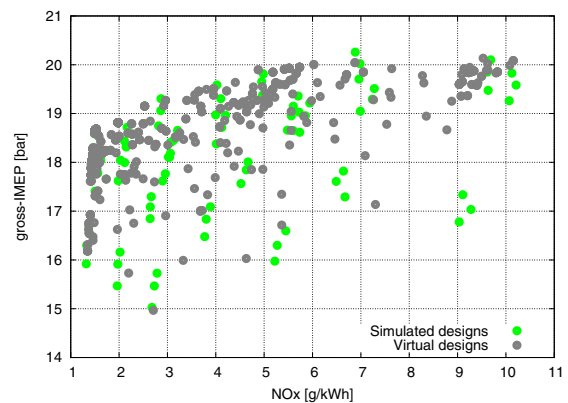
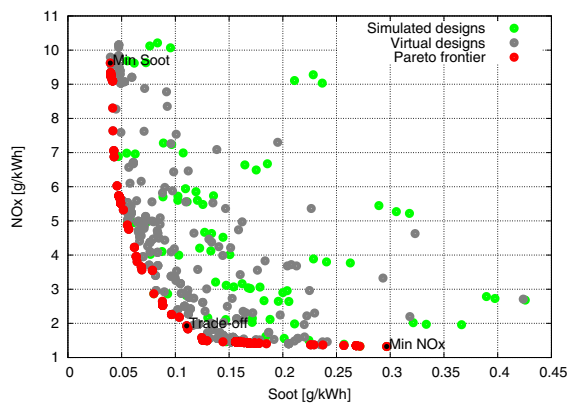


Fig. 4. (a) Bowl A soot - NO_x; (b) Bowl A NO_x - IMEP

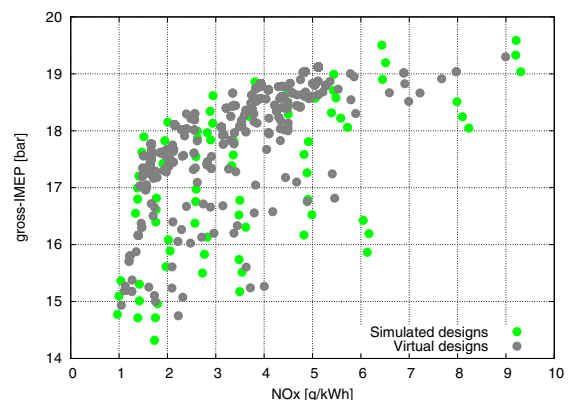
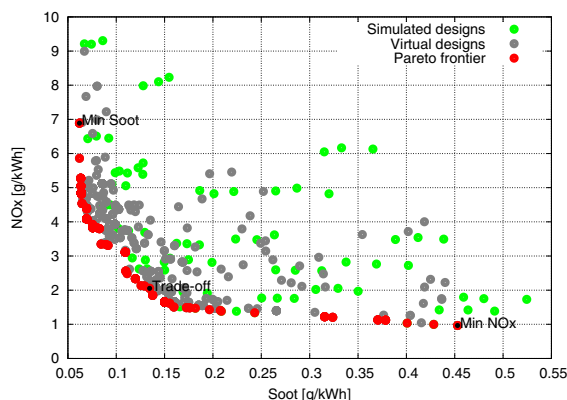


Fig. 5. (a) Bowl B soot - NO_x; (b) Bowl B NO_x - IMEP

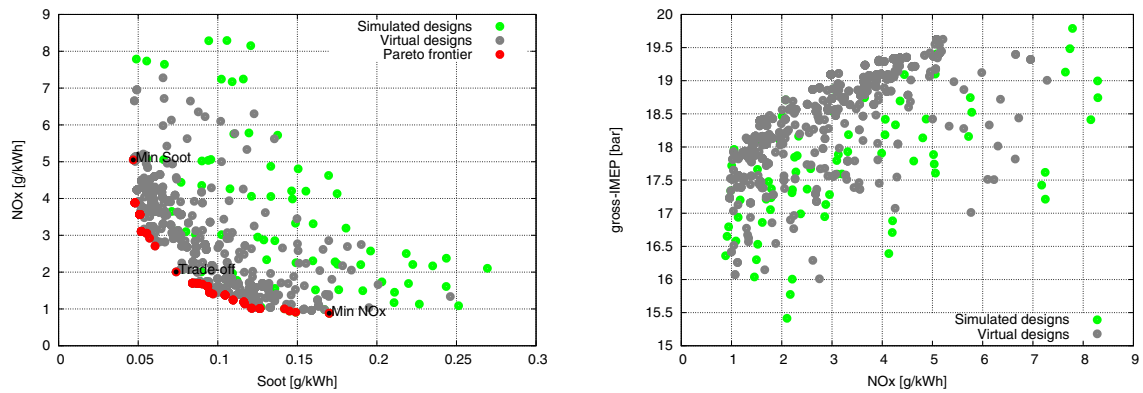


Fig. 6. (a) Bowl C soot - NOx; (b) Bowl C NOx - IMEP

Amongst the Pareto optimal solutions, it was also possible to find the minimum NOx individuals, the minimum soot individuals and the trade-off individuals whose input parameters are reported in table 4.

Table 4. Trade-off individuals

Bowl	P_{boost}	SR	EGR	SOI
A	3.39	1.5	13.0	-6.6
B	3.33	1.3	12.0	-6.0
C	3.39	1.6	10.0	-6.0

8. Validation of the best individuals

Figure 7 shows a comparison between the Pareto frontiers of the piston bowl A, B and C in the soot-NOx plane. As it can be seen, the Pareto frontier of the piston bowl C lies south-west than the other ones which means that its individuals will have a lower soot emission for a given NOx emission, otherwise, will have a lower NOx emission for a given soot emission.

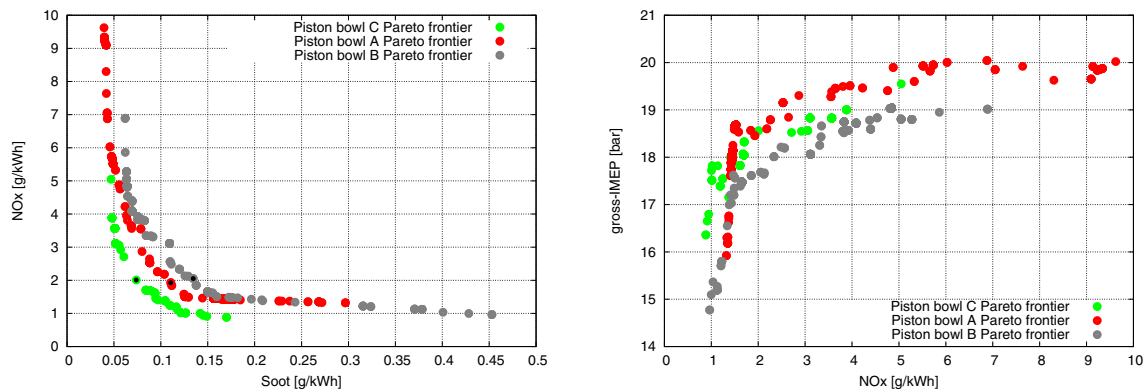


Fig. 7. (a) Pareto frontiers soot-NOx; (b) Pareto frontiers NOx-IMEP

Amongst the Pareto optimal solutions, one individual for each piston bowl (represented as a black dot in figure 7 (a)) was chosen as the optimal solution and was, thus, validated by means of an actual CFD three-dimensional combustion simulation.

In table 5 are reported the comparisons between the values of NO_x, soot and gross-IMEP foreseen by means of the RBF neural networks and the actual values, resulting from CFD calculations of the best individuals. For all the three investigated piston bowls, the greatest relative error (about 10%) was made evaluating NO_x emissions. Particularly, as far as NO_x emissions were concerned, all the trade-off individuals recorded a lower emission than the one foreseen by the RBF neural network. On the contrary, a very good agreement between neural networks and CFD results was found both for soot emission, where a maximum relative error of 7.7% was recorded, and gross-IMEP, for which a maximum error of 2.8% was recorded.

Table 5. Validation of the best individuals

Piston bowl	NO _x [g/kWh]	Soot [g/kWh]	IMEP [bar]
A	1.7 (-10.5%)	0.11 (-0.0%)	18.9 (+2.2%)
B	1.8 (-10.0%)	0.12 (-7.7%)	18.2 (+2.8%)
C	1.8 (-10.0%)	0.07 (-0.0%)	18.9 (+1.6%)

Finally, emissions and performance results of the optimal solutions, evaluated by means of actual CFD three-dimensional combustion calculations, were compared in order to point out the best piston bowl shape for the investigated engine. It can be seen (table 6) how the piston bowl C allowed a decrease of soot emission of about -36% with approximately the same NO_x emission and gross-IMEP of the piston bowl A which represented the baseline design of the engine.

Table 6. Best individuals emissions and performance

Piston bowl	NO _x [g/kWh]	Soot [g/kWh]	IMEP [bar]
A	1.7	0.11	18.9
B	1.8 (+5%)	0.12 (+9%)	18.2 (-4%)
C	1.8 (+5%)	0.07 (-36%)	18.9 (-0%)

9. Conclusion

In order to achieve a significant combustion improvement it is mandatory, for the future DI Diesel engine, to develop a robust design methodology focused on decreasing NO_x and soot emissions simultaneously while maintaining a reasonable fuel economy. For this kind of problem, multi-objective genetic algorithms have been successfully used, over the last few years, due to their ability to find multiple Pareto-optimal solutions in one single run moving the Pareto front towards the ideal optimal set of solutions as the optimization process evolves. Nonetheless, combining GAs optimization with actual CFD three-dimensional combustion simulations can be too onerous since a large number of calculations is usually needed for the genetic algorithm to converge, resulting in a high computational cost and, thus, limiting the suitability of this method for industrial processes.

In the current work, a numerical methodology for the multi-objective virtual optimization of the combustion of an automotive DI Diesel engine, which relies on artificial neural networks and genetic algorithms, was developed.

The proposed methodology was used to aid the development process of a VM Motori DI Diesel engine targeted for automotive applications allowing to evaluate three different piston bowls under a wide range of operating conditions and to find out, for each piston bowl, the Pareto-optimal individuals with a small number of calculations. At the final stage of the work, the best solutions were validated through actual CFD three-dimensional calculations and the best piston bowls, together with its set of optimal input parameters, was found out allowing to decrease soot emission of about -36% with approximately the same NO_x emission and gross-IMEP.

Finally, the developed numerical methodology proved to be both fast, decreasing the computational cost needed for each optimization from approximately 2100 hours to approximately 24 hours on a 8 Intel Xeon core @ 2.4 GHz computer, and accurate and, thus, is currently successfully used to aid the development of several DI Diesel engine.

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